

****Volume Title****

*ASP Conference Series, Vol. **Volume Number***

****Author****

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Infrared Opacities in Dense Atmospheres of Cool White Dwarf Stars

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Abstract.

Dense, He-rich atmospheres of cool white dwarfs represent a challenge to the modeling. This is because these atmospheres are constituted of a dense fluid in which strong multi-atomic interactions determine their physics and chemistry. Therefore, the ideal-gas-based description of absorption is no longer adequate, which makes the opacities of these atmospheres difficult to model. This is illustrated with severe problems in fitting the spectra of cool, He-rich stars. Good description of the infrared (IR) opacity is essential for proper assignment of the atmospheric parameters of these stars. Using methods of computational quantum chemistry we simulate the IR absorption of dense He/H media. We found a significant IR absorption from He atoms (He-He-He CIA opacity) and a strong pressure distortion of the H₂-He collision-induced absorption (CIA). We discuss the implication of these results for interpretation of the spectra of cool stars.

1. Introduction

Atmospheres of old and cool white dwarfs deliver valuable information on stellar and planetary evolution. This is because of relatively simple cooling physics that allows for accurate cosmochemistry (Richer et al. 2006; Fontaine et al. 2001) and of the stratified nature of a white dwarf star, which allows for tracing the content of accreted planetary-like material (Farihi et al. 2010). However, in order to properly assess this information, atmospheres of these stars must be well characterized and understood. This is often difficult with the standard models that are based mainly of the ideal-gas description of physics and chemistry. The atmospheres of helium-rich stars reach densities of fluid (up to a few g/cc (Kowalski 2006a, 2010; Bergeron et al. 1997)) and there are severe problems in proper characterization of such old stars (e.g. Gianninas et al. (2015)). Impact of the dense atmospheres on stellar spectra are illustrated by the pressure distortion of C₂ bands (Schmidt et al. 1995; Bergeron et al. 1997; Kowalski 2010) and also with some problems with fitting the metal lines profiles (Dufour et al. 2007). The former problems in fitting the UV spectra and U and B photometric bands of less extreme hydrogen-rich white dwarfs (Bergeron et al. 1997), solved by introduction of the Ly- α red wing opacities (Kowalski & Saumon 2006; Kowalski 2006b), also show the importance of proper modeling, accurate fitting and characterization of spectra of cool white dwarfs, for correct understanding of these stars (Saumon et al. 2014).

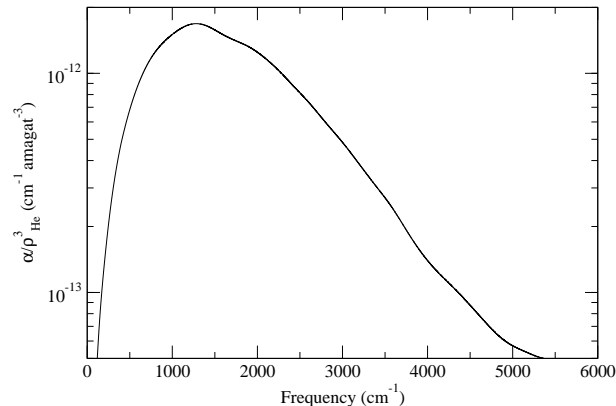


Figure 1. Simulated IR absorption profile of dense helium obtained for $T = 5000$ K (Kowalski 2014). The densities are expressed in amagat = $2.68678 \cdot 10^{19} \text{ cm}^{-3}$.

In the last two decades various high-pressure improvements have been introduced to the modeling. These include the non-ideal equation of state (Saumon & Jacobson 1999), the opacities (Iglesias et al. 2002; Kowalski 2010, 2014; Kowalski & Saumon 2006; Kowalski 2006b), the refraction (Kowalski & Saumon 2004) and the chemical abundances of species (Kowalski 2006a). The further tests of Ly-alpha red wing profiles validated this absorption mechanism for a sample of cool stars (Saumon et al. 2014). While the less extreme atmospheres of hydrogen-rich white dwarfs are now well reproduced by the current models, the modeling of more extreme helium-rich atmospheres still encounters difficulties (Kowalski et al. 2013; Gianninas et al. 2015). In spite of significant work devoted to improvement of high density chemistry and physics description, no conclusive models describing dense, helium-rich atmospheres exist. In particular, a group of so-called ultracool white dwarfs, which are believed to be helium-rich stars, have rather vague atmospheric parameters assignment (Gianninas et al. 2015). We suspect that the pressure-distortion of IR opacities, namely the collision induced absorption (CIA, Frommhold (1993)), contributes to much of these difficulties.

Having steady improvement in the performance and availability of the computational power and quantum chemistry simulation software and techniques, many dense helium problems could be tackled by atomistic simulations (Jahn & Kowalski 2014). The IR opacities could be directly simulated using *ab initio* methods of quantum chemistry (Guillot 1991; Silvestrelli et al. 1997; Jahn & Kowalski 2014). Recently we attempted such simulations and the first results are briefly discussed here in the context of interpreting the near- and mid-IR spectra of ultracool stars.

2. He-He-He CIA opacity

Recently, using *ab initio* molecular dynamics technique, Kowalski (2014) simulated the CIA opacities of pure, dense helium and found significant absorption resulting from triple collisions between helium atoms. This absorption mechanism was postulated (e.g. Frommhold (1993)), but had been never before observed experimentally or computed. The obtained absorption coefficient for a representative temperature of 5000

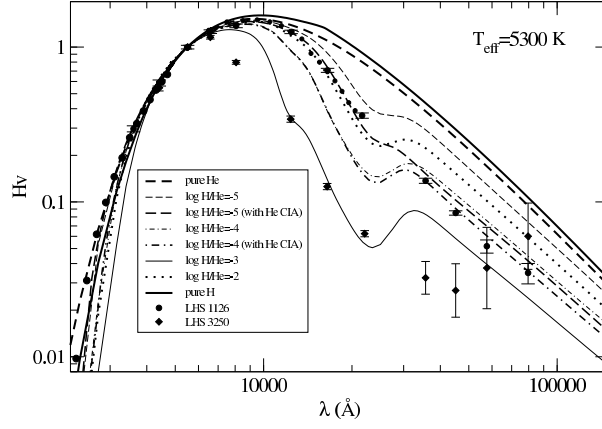


Figure 2. Comparison of the SED of the He-rich stars LHS 1126 and LHS 3250 with models of different H/He atmosphere composition, $T_{\text{eff}} = 5300$ K and $\log g = 8$. The photometric fluxes are from Bergeron et al. (2001), Kilic et al. (2008) and Kilic et al. (2009). For LHS 1126 the UV flux is from Wolff et al. (2002) and the near-IR flux is our new data (Kowalski et al. 2013). All the spectra are normalized to the V band flux. The thick long dashed and dot-dashed lines represent the models with the He-He-He CIA opacity.

K is given in Figure 1. Although the intensity of this absorption mechanism is about four orders of magnitude lower than the relevant $\text{H}_2/\text{H-He}$ CIA opacities, because He atoms are the dominant species it becomes a significant IR absorption mechanism in the atmospheres with $\text{He}/\text{H} > 10^4$ (see Fig. 2). When we applied the new absorption mechanism to the spectrum of LHS1128 star, which is broadly discussed by Kowalski et al. (2013) (Fig. 2), we obtained much better fit to the IRAC fluxes. This opacity source thus explains a flat-like behavior of the observed IR fluxes, as opposite to the $2.3 \mu\text{m}$ flux suppression and the $3.5 \mu\text{m}$ flux excess predicted by the current models (Fig. 2).

3. H_2 -He CIA opacities

Using the same simulation method as Kowalski (2014) used for simulation of the He-He-He absorption (see also Blouin et al. (2017) in this volume) we have simulated the $\text{H}_2 - \text{He}$ CIA opacities. As indicated in Fig. 2 of Blouin et al. (2017) we found a significant distortion of this absorption mechanism for densities $\rho > 0.1$ g/cc. The obtained profiles for the low and high densities are compared in Figure 3. As indicated in the figure, there are three main pressure effects. (1) The rototranslational band peak at $\sim 1000 \text{ cm}^{-1}$ becomes more pronounced and (2) shifted towards higher frequencies. We interpret this as a result of triple collisions (Lenzuni & Saumon 1992) and decrease in the separation between hydrogen atoms in H_2 with increase in density, and related decrease of the H_2 rotational inertia, as illustrated in Fig. 4. At the same time, (3) the $\sim 4200 \text{ cm}^{-1}$ main vibrational band shifts to the higher frequencies and splits into two peaks due to an interference between the dipole moments induced in the successive collisions of H_2 and He atoms (Kranendonk 1968). This splitting has been experimentally observed before (Hare & Welsh 1958) and in Figure 5 we compare those results

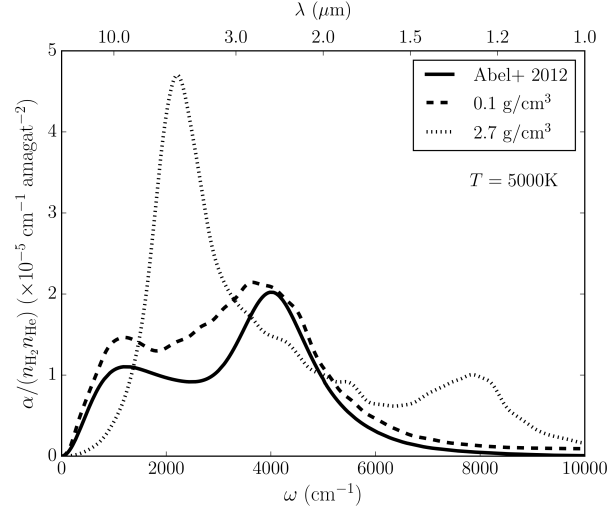


Figure 3. The comparison of the simulated $\text{H}_2 - \text{He}$ CIA opacities at low and high densities. Note that the results of Abel et al. (2012), plotted here as a reference, are not corrected for high density (triple collisions, Lenzuni & Saumon (1992)), and should be thus underestimated by $\sim 30\%$ at $\rho = 0.1 \text{ g/cc}$.

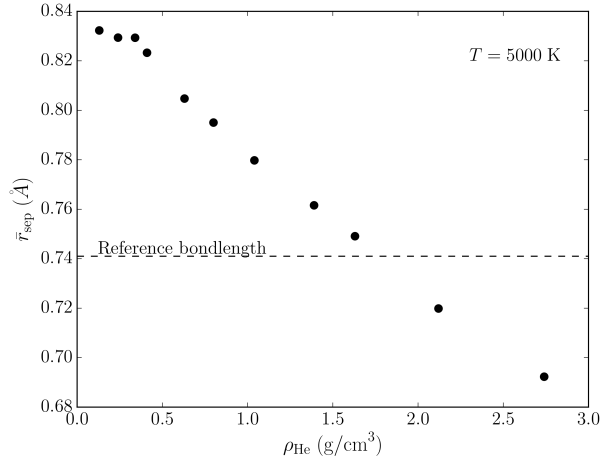


Figure 4. The simulated average interatomic separation in H_2 molecule as a function of density.

with these simulated by us. We obtained larger splitting because simulations were performed at much higher temperature, thus with higher thermal collisions energy than in the experiments performed at ambient conditions.

The obtained results could be used for the interpretation of difference between the modeled and the observed spectra of ultracool white dwarfs, such as LHS3025. Compared to the synthetic spectrum computed using the standard CIA opacity descrip-

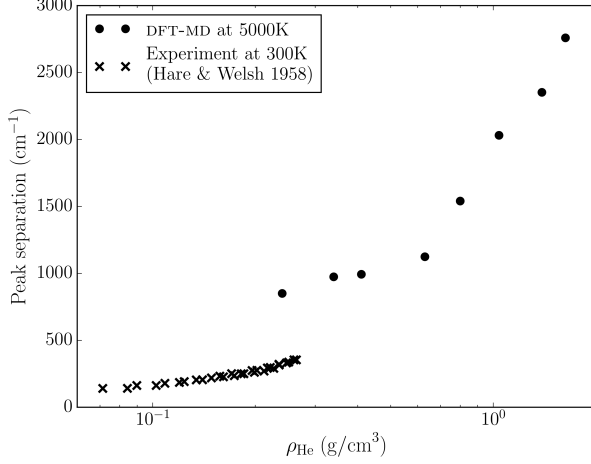


Figure 5. The main vibrational peak separation as a function of density. The different symbols represent the values simulated here and the experimental results of Hare & Welsh (1958).

tion of Abel et al. (2012), the observed spectrum does not show the clear minimum at $2.3\mu\text{m}$ and the flux excess at $\sim 3.5\mu\text{m}$ that are predicted by models, and indicates more absorption in the near-IR. This is consistent with the simulated broadening and the redistribution of the main vibrational peak and the enhancement of rototranslational peak. The absorption spectrum simulated at $\rho = 2.7\text{ g/cc}$ (Fig. 3) indicates maximum of absorption at $\sim 5\mu\text{m}$ and more absorption in the near-IR, which is consistent with the observed spectral energy distribution of LHS3025, and also other ultracool white dwarfs (Gianninas et al. 2015). More elaborate analysis requires more complete set of simulated spectra, including investigation of the temperature dependence, derivation of the relevant distortion model, calculations of a grid of atmosphere models and their usage for subsequent fitting of spectra and analysis of ultracool white dwarfs. This work is currently in progress.

4. Conclusion

We have showed the results of simulations of He-He-He and H₂-He CIA infrared opacities and their impact for the interpretation of spectra of cool, helium-rich stars, including ultracool white dwarfs. We discuss the impact of the newly found He-He-He CIA opacity from pure helium on the spectra. By improved fit to the spectrum of LHS1128 star we show that this opacity mechanism could be responsible for a flat-like infrared spectral energy distribution of these stars, which could not be reproduced with previous models. The subsequent simulations of H₂-He CIA opacities show significant pressure-distortion of this absorption mechanism with the simulated intensity change being consistent with the one deduced from the mismatch between the current models prediction and the observed spectral energy distribution for star LHS3250. However, more complete simulations of the IR opacities and subsequent computation of new models are required for complete analysis and refitting the spectra of cool, helium-rich stars, which is currently in progress. Last but not least, the simulations conducted here

and the subsequent analysis show that the modern atomistic modeling methods could be successfully applied to modeling condensed stellar atmospheres and that, on the other hand, the atmospheres of white dwarfs represent excellent laboratories for testing the physics and chemistry of matter at extreme conditions.

Acknowledgments. S.B. acknowledges support from NSERC (Canada), FRQNT (Québec) and DAAD (Germany).

References

- Abel, M., Frommhold, L., Li, X., & Hunt, K. L. C. 2012, *The Journal of Chemical Physics*, 136, 044319
- Bergeron, P., Leggett, S. K., & Ruiz, M. T. 2001, *ApJ*, 133, 433
- Bergeron, P., Ruiz, M. T., & Leggett, S. K. 1997, *ApJ*, 108, 339
- Blouin, S., Dufour, P., & Kowalski, P. M. 2017 (*Astronomical Soc. of the Pacific*), vol. This volume
- Dufour, P., Bergeron, P., Liebert, J., Harris, H. C., Knapp, G. R., Anderson, S. F., Hall, P. B., Strauss, M. A., Collinge, M. J., & Edwards, M. C. 2007, *The Astrophysical Journal*, 663, 1291
- Farihi, J., Barstow, M. A., Redfield, S., Dufour, P., & Hambly, N. C. 2010, *Mon. Not. R. Astron. Soc.*, 404, 2123
- Fontaine, G., Brassard, P., & Bergeron, P. 2001, *PASP*, 113, 409
- Frommhold, L. 1993, *Collision-induced Absorption in Gases* (Cambridge University Press)
- Gianninas, A., Curd, B., Thorstensen, J. R., Kilic, M., Bergeron, P., Andrews, J. J., Canton, P., & Agueros, M. A. 2015, *Monthly Notices of the Royal Astronomical Society*, 449, 3966
- Guillot, B. 1991, *The Journal of Chemical Physics*, 95
- Hare, W. F. J., & Welsh, H. L. 1958, *Canadian Journal of Physics*, 36, 88
- Iglesias, C. A., Rogers, F. J., & Saumon, D. 2002, *The Astrophysical Journal Letters*, 569, L111
- Jahn, S., & Kowalski, P. 2014, *Reviews in mineralogy & geochemistry*, 78, 691
- Kilic, M., Kowalski, P. M., Mullally, F., Reach, W. T., & von Hippel, T. 2008, *ApJ*, 678, 1298
- Kilic, M., Kowalski, P. M., Reach, W. T., & von Hippel, T. 2009, *ApJ*, 696, 2094
- Kowalski, P. 2014, *A&A*, 566, L8
- Kowalski, P., Saumon, D., Holberg, J., & Leggett, S. 2013 (*San Francisco, Calif.: Astronomical Soc. of the Pacific*), 173
- Kowalski, P. M. 2006a, *The Astrophysical Journal*, 641, 488
- 2006b, *The Astrophysical Journal*, 651, 1120
- 2010, *A&A*, 519, L8
- Kowalski, P. M., & Saumon, D. 2004, *The Astrophysical Journal*, 607, 970
- 2006, *ApJ*, 651, L137
- Kranendonk, J. V. 1968, *Canadian Journal of Physics*, 46, 1173
- Lenzuni, P., & Saumon, D. 1992, *Revista Mexicana de Astronomia y Astrofisica*, 23, 223
- Richer, H. B., Anderson, J. B., James, D. S., Fahlman, G. G., Hansen, B. M. S., Hurley, J., Kalirai, J. S., King, I. R., Reitzel, D., Rich, R. M., Shara, M. M., & Stetson, P. B. 2006, *Science*, 313, 936
- Saumon, D., Holberg, J. B., & Kowalski, P. M. 2014, *The Astrophysical Journal*, 790, 50
- Saumon, D., & Jacobson, S. B. 1999, *The Astrophysical Journal Letters*, 511, L107
- Schmidt, G. D., Bergeron, P., & Fegley, B. 1995, *ApJ*, 443, 274
- Silvestrelli, P. L., Bernasconi, M., & Parrinello, M. 1997, *Chemical Physics Letters*, 277, 478
- Wolff, B., Koester, D., & Liebert, J. 2002, *A&A*, 385, 995